SUPPPORTING INFORMATION

Crystal Structures, Metal-activation and DNA-binding Properties of Two-domain IdeR from *Mycobacterium tuberculosis*

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Table S1 Equilibrium constants for metal ion activation of 2D-IdeR for binding to the *fxbA* operator

Metal ion	$\langle K_d \rangle^a$ **(μM)**	$\langle K_d \rangle^a$ **for full-length IdeR**^{b} **(μM)**
Co^{2+}	24.7 ± 1.1	22.6 ± 1.9
Ni^{2+}	4.3 ± 1.0	13.1 ± 0.1

[a] The average value of at least three titrations.
[b] Data from Chou *et al.* (*14*)

Table S2 Metal-ligand distances (Å) for all metal-binding sites

			2D-IdeR		2D-IdeR:DNA complex (crystal form I)				2D-IdeR:DNA complex (crystal form II)			
Site	Residue	Atom	**A**	**B**	**A**	**B**	**C**	**D**	**A**	**B**	**C**	**D**
Ni 1	His79	$N^{\varepsilon 2}$	2.22	2.08	2.04	2.03	2.04	2.03	2.02	2.01	2.01	2.02
	Glu83	$O^{\varepsilon 2}$	2.14	2.11	1.96	1.96	1.96	1.96	1.95	1.95	1.94	1.94
	His98	$N^{\delta 1}$	2.15	2.11	2.04	2.05	2.04	2.03	2.02	2.02	2.03	2.00
	Phosphate	O^{1}	2.17	2.25	-	-	-	-	-	-	-	-
	H_2O (1)	O	2.19	2.08	2.60	2.61	-	2.62	-	-	-	-
	H_2O (2)	O	2.37	2.19	-	-	-	-	-	-	-	-
	Acetate (1)	O	-	-	-	-	-	-	2.12	2.49	2.17	2.48
	Acetate (1)	O^{XT}	-	-	-	-	-	-	2.35	2.45	2.27	1.87
Ni 2	Met10	S^{δ}	2.42	2.47	2.37	2.33	2.36	2.34	2.34	2.33	2.35	2.34
	Cys102	O	2.15	2.08	1.97	1.96	1.95	1.95	1.96	1.95	1.94	1.95
	Cys102	S^{γ}	-	-	2.79	2.61	2.85	3.08	2.75	2.73	2.78	2.81
	Cys102[a]	O^{1}	1.91	2.11	-	-	-	-	-	-	-	-
	Glu105	$O^{\varepsilon 2}$	2.04	2.12	1.95	1.95	1.96	1.95	1.94	1.94	1.94	1.94
	His106	$N^{\varepsilon 2}$	2.07	1.98	2.03	2.04	2.02	2.04	2.02	2.03	2.02	2.01
	H_2O	O	2.21	2.18	1.99	2.98	2.31	2.27	-	-	2.33	-
Ni 3	His61	$N^{\delta 1}$	-	-	2.03	2.03	2.02	2.03	2.02	2.03	2.03	2.01
	H2O	O	-	-	-	1.83	2.07	2.67	-	-	-	-
	H2O	O	-	-	-	2.32	2.44	2.74	-	-	-	-
	H2O	O	-	-	-	2.33	2.85	-	-	-	-	-
	Acetate (2)	O	-	-	-	-	-	-	2.21	1.93	2.39	2.42
	Acetate (2)	O^{XT}	-	-	-	-	-	-	2.87	2.07	2.48	1.97
	Acetate (3)	O	-	-	-	-	-	-	2.08	-	2.66	-
	Acetate (3)	O^{XT}	-	-	-	-	-	-	2.74	-	2.50	-
Na	Phosphate	O^{2P}	-	-	2.86[b] (*F*19)	-	3.24[b] (*E*16)	3.17[b] (*F*24)	-	-	-	-
	H_2O (1)	O	-	-	1.86	-	2.28	1.94	-	-	-	-
	H_2O (2)	O	-	-	2.00	-	2.49	2.12	-	-	-	-
	H_2O (3)	O	-	-	2.10	-	2.54	2.35	-	-	-	-
	H_2O (4)	O	-	-	2.24	-	-	-	-	-	-	-

[a]Cys 102 is modeled as S-hydroxy cystein in 2D-IdeR structure.
[b]Phosphate oxygen of residues in parenthesis coordinate to sodium ions.

Table S3 Distance (Å) between Ser37/Pro39 and interacting nucleotide bases (with a 3.9 Å cutoff distance) in the 2D-IdeR:DNA complex structures

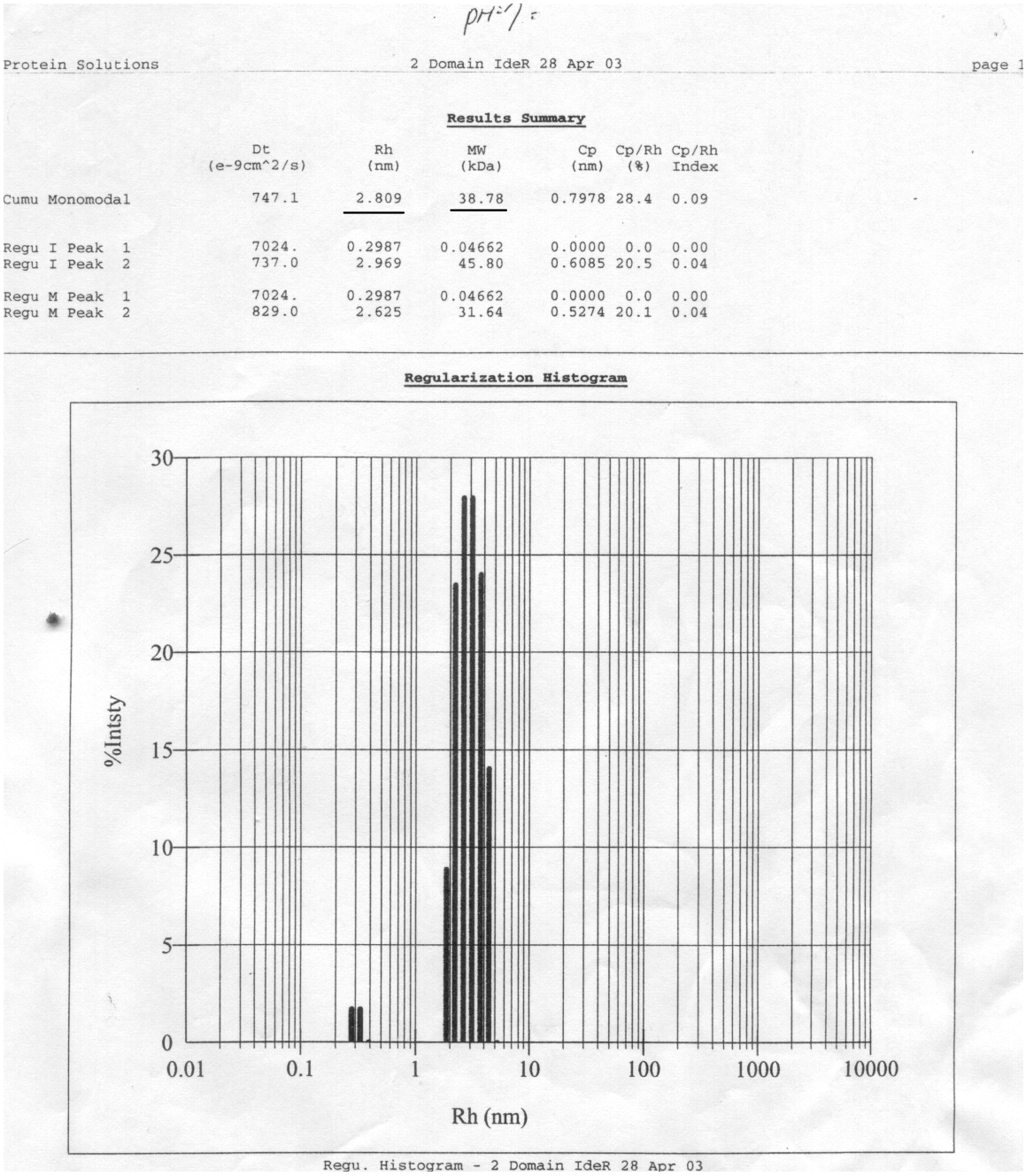
IdeR subunit	**A**			**B**				**C**			**D**			
Nucleotide (chain)	*T20* (**F**)	*G21* (**F**)	*C12* (**E**)	*T22* (**E**)	*A23* (**E**)	*T10* (**F**)	*T9* (**F**)	*T17* (**E**)	*G18* (**E**)	*C15* (**F**)	*T25* (**F**)	*A26* (**F**)	*T7* (**E**)	*T6* (**E**)
Crystal form I														
Ser37 C^{β}	3.49 (C5M)	-	-	3.55 (C5M)	-	-	-	3.42 (C5M)	-	-	3.47 (C5M)	-	-	-
Ser37 O^{γ}	3.38 (C5M)	-	-	3.40 (C5M)	-	-	-	3.44 (C5M)	-	-	3.34 (C5M)	-	-	-
Pro39 N	-	-	-	-	-	-	3.50 (C5M)	-	-	-	-	-	-	3.74 (C5M)
Pro39 C^{α}	-	-	-	-	-	-	3.80 (C5M)	-	-	-	-	-	-	-
Pro39 C^{β}	3.09 (O4)	-	-	3.49 (O4)	-	3.46 (O4)	-	3.27 (O4)	-	-	3.41 (O4)	-	-	-
Pro39 C^{γ}	2.97 (O4) 3.65 (C5M)	3.58 (O6)	3.68 (N4)	3.34 (O4)	3.51 (N6)	3.19 (O4)	3.70 (O4)	2.98 (O4) 3.71 (C5M)	3.87 (O6)	3.70 (N4)	3.26 (O4)	3.57 (N6)	3.47 (O4)	3.78 (O4)
Pro39 C^{δ}	3.82 (C5M)	-	-	-	-	-	3.85 (O4) 3.86 (C5M)	3.75 (C5M)	-	-	-	-	-	-
Crystal form II														
Ser37 C^{β}	3.49 (C5M)	-	-	3.28 (C5M)	-	-	-	3.34 (C5M)	-	-	3.56 (C5M)	-	-	-
Ser37 O^{γ}	3.57 (C5M)	-	-	3.35 (C5M)	-	-	-	3.29 (C5M)	-	-	3.22 (C5M)	-	-	-
Pro36 N	-	-	-	-	-	-	3.82 (C5M)	-	-	-	-	-	-	-
Pro39 C^{β}	3.30 (O4)	-	3.85 (N4)	3.39 (O4)	-	3.49 (O4)	-	3.13 (O4)	-	-	3.37 (O4)	-	3.74 (O4)	-
Pro39 C^{γ}	3.30 (O4) 3.89 (C5M)	3.89 (O6)	3.54 (N4)	3.33 (O4)	3.18 (N6)	3.40 (O4)	3.46 (O4)	3.18 (O4)	3.74 (O6)	3.71 (N4)	3.31 (O4) 3.74 (C5M)	3.42 (N6)	3.57 (O4)	-
Pro39 C^{δ}	-	-	-	-	-	-	3.76 (O4)	-	-	-	-	-	-	-

Table S4 Distance (Å) between selected atoms of Gln43 and interacting nucleotide bases (with a 3.9 Å cutoff distance) in the 2D-IdeR:DNA complex structures

IdeR subunit	**A**		**B**		**C**[a]		**D**	
Nucleotide (chain)	*C*17 (**F**)	*C*18 (**F**)	*C*19 (**E**)	*C*20 (**E**)	*G*14 (**E**)	*G*15 (**E**)	*T*22 (**F**)	*G*23 (**F**)
Crystal form I								
Gln43 C^{δ}				3.70 (N4)				
Gln43 $O^{\varepsilon 1}$	-	3.83 (C4) 3.07 (N4) 3.71 (C5)	3.68 (C5)	3.50 (C4) 2.70 (N4) 3.48 (C5)	-	-	-	-
Gln43 $N^{\varepsilon 2}$	-	-	-	-	-	-	-	-
Crystal form II								
Gln43 C^{δ}				3.86 (N4)				
Gln43 $O^{\varepsilon 1}$	3.65 (N7)	3.38 (N4) 3.81 (C5)	3.52 (C5)	3.66 (C4) 2.81 (N4) 3.65 (C5)	-	-	-	-
Gln43 $N^{\varepsilon 2}$	-	-	-	-	-	-	-	-

[a]Gln43 of subunit C in crystal form II makes the following unusual contacts to nucleotide bases:
Gln43 $O^{\varepsilon 1}$ - *C*16**E** N4 (3.23 Å) and Gln43 $N^{\varepsilon 2}$ - *G*17**F** O6 (3.35 Å)

Figure S1 Representative dynamic-light scattering data



pH 7.5

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Results Summary

	Dt (e-9cm^2/s)	Rh (nm)	MW (kDa)	Cp (nm)	Cp/Rh (%)	Cp/Rh Index
Cumu Monomodal	747.1	2.809	38.78	0.7978	28.4	0.09
Regu I Peak 1	7024.	0.2987	0.04662	0.0000	0.0	0.00
Regu I Peak 2	737.0	2.969	45.80	0.6085	20.5	0.04
Regu M Peak 1	7024.	0.2987	0.04662	0.0000	0.0	0.00
Regu M Peak 2	829.0	2.625	31.64	0.5274	20.1	0.04

Regularization Histogram

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